III.D.1 An Integrated Approach to Modeling and Mitigating SOFC Failure

Objectives

- Generate new scientific and engineering knowledge to better enable SECA industry teams to develop low-cost solid-oxide fuel cell power generation systems.
- Create technology breakthroughs to address technical risks and barriers that currently limit achievement of the SECA performance and cost goals for solid-oxide fuel cell systems.
- Transfer new science and technology developed in the Core Technology Program to the SECA industry teams.

Accomplishments

- Developed and implement a suitable failure effects analysis (FEA) tool for analysis of fracture failure in the context of various pre-existing flaws within SOFC cells under various operating conditions. The program Fracture Mechanical Analyzer (FMA) was developed and transferred to SECA.
- Developed higher order (second and third) analytical model of the SOFC heating/cooling during start-up/shut-down in the limit of optically thin anode-electrolyte-cathode (PEN) layers assembly and local thermal equilibrium between the layers.

Introduction

It is well known that thermal transients and gradients impose states of stress within SOFC cell materials that may result in crack initiation, propagation and subsequent structural failure or performance degradation in short-term operation; furthermore, due to a variety of mechanisms, performance may significantly decrease over time. The commercial viability of SOFC power generation systems is dependent upon making significant progress in the durability and reliability of cell and stack structures. However, no systematic study of the causes or physical drivers of cell failure and degradation have been conducted; as a result, no coherent degradation or useful life prediction modeling methodology is currently available. A new modeling methodology could significantly contribute to efficient development of SECA SOFC system performance requirements.

Additionally, previous modeling attempts to characterize SOFC failure modes have been limited because of simplified transport models. One dimensional, "bulk" electrochemical and thermal models have been applied, and these models have been decoupled (i.e., interdependency between electrochemistry and thermal transport neglected). In order to create greater fidelity within thermomechanical failure analysis models, interdependency between structural issues and electrochemical/thermal transport phenomena must be characterized. This requires a multi-physics modeling approach as demonstrated in this research.

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Approach

The recent shift of SOFCs to anode-supported structures, in which a thin film electrolyte is sintered onto the anode support, has further hampered structural modeling due to the large aspect ratio between the anode/electrolyte layers and cell length. Yet due to thermal mismatch between these layers and the cell operating conditions, significant thermal stresses are created within the cell structure, which may eventually lead to failure, making fracture analysis a critical part of thermomechanical modeling of SOFCs. Specifically, simulation tools are needed to obtain fracture mechanics parameters, such as the stress intensity factors (SIFs), and to understand the influence of thermal gradients on crack behavior.

To meet this need, a computer program called Fracture Mechanical Analyzer (FMA) was developed to calculate the SIFs of 3-D cracks, including interfacial cracks in the PEN structure subjected to combined mechanical and thermal loadings [1-3]. The FMA program, written in MatLab language, is essentially an "add-on" to any commercial finite element software. It computes the energy release rate and the individual SIFs based on the crack-tip displacement fields computed from any commercial finite element software.

Additionally new models were developed to analyze the thermal behavior in SOFCs and transient modeling of the SOFC unit cell is a prerequisite to mitigating

thermo-mechanical failure caused by thermal gradients and cycling at start-up/shut-down. At start-up, it is desirable to heat the cell as quickly as possible under the constraint of some maximum allowable temperature gradient. Thermal modeling focused on correlating the heating rate and the observed temperature gradients, and was presented in a manner that easily yields this information for the cell designed.

Three models of increasing complexity and accuracy were developed. The first two models assume that the cell is thermally thin, that is, the cell materials have high thermal diffusivity so thermal field development in the solid intimately follows that in the heating air. The third model relaxes this assumption and gives consideration to the thermal resistance and latency (thermal energy storage) of the cell materials. Results from these models were compared to the transient solution obtained by the fully 3-D transient Fluent model to identify the "best" model featuring the least degree of complexity and computational expense yet resulting in sufficient accuracy of simulation results.

Results

The 3-D structural analysis was separated into two steps: a global cell model and a local fracture model. The global–local modeling technique extrapolated the boundary displacements and temperature fields from a location in the full-scale model to the smaller local fracture model. This fracture model would be able to incorporate a higher density of nodes at the crack edge over that of a full-scale model featuring a crack. Fracture parameters were then determined by using the FMA program.

Figure 1 is a diagram of the global model used for analysis, Figure 2 is an example of the normalized stress curve seen in the model for a given set of boundary conditions, and Figure 3 is a plot of the SIF of a vertical penny crack in the anode versus differing electrolyte heights. The stress intensity factor plotted is KI which means a tensile stress is seen in the anode during cool down from operation such that if the temperature change was high enough the crack would grow upwards to the electrolyte. This model assumed a temperature drop of 200°C which was not sufficient for crack growth.

In the thermal analysis after reviewing the results and analysis of the simplified analytical transient heating models and the numerical, 2-equation, non-equilibrium model, guidance was provided concerning model selection and limits of applicability. Thermal

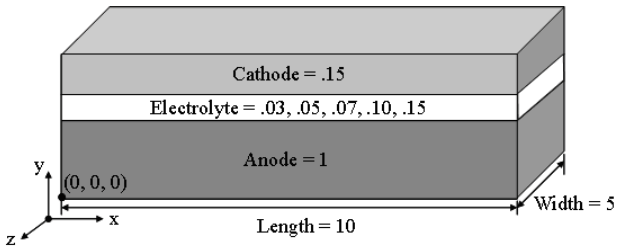

FIGURE 1. Model Configuration for PEN Layer

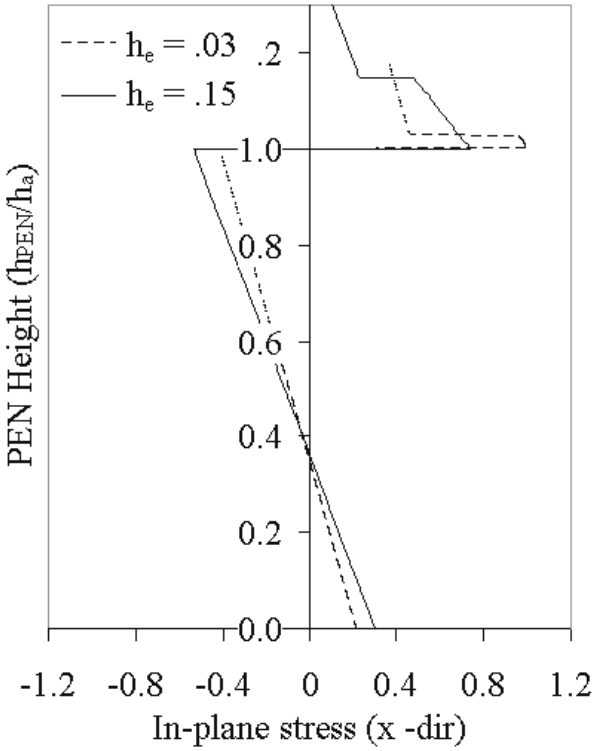

FIGURE 2. In-Plane Stress for Positive Temperatures versus PEN Height

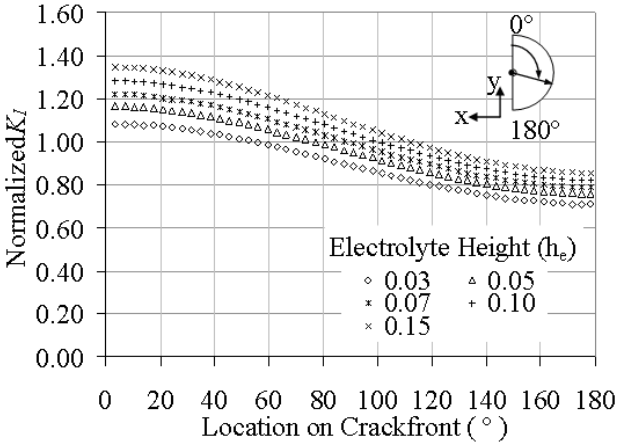

FIGURE 3. Mode I SIF for Crack in Anode for Different Electrolyte Heights with Crack Center at (2.5, 0.6, 0)

modeling efforts thus far have focused on correlating the heating rate and the observed temperature gradients in a unit cell heated by flowing hot air into the oxidizer channel. The linear rate of temperature rise, *K*, and mean velocity, *U*, of the heating air are design variables that can be controlled in maintaining temperature gradients below a given threshold while minimizing heating time requirements. In the analysis of each simplified model, the predictions of heating time and maximum temperature gradient developed in the cell were compared to results from 3-D, computational fluid dynamics (CFD) Fluent model simulations. Thus, we assessed the capability of these models to predict these *global* quantities while making no judgment concerning the ability of the models to accurately predict *detailed* time-varying temperature fields.

The model predicts heating time and temporal temperature gradient to a high degree of accuracy (~2% error) compared to CFD results. Model predictions of maximum spatial temperature gradient (along the flow direction) are less precise (< 20% error). For the values of *K* and *U* given, the 1st and 2nd order models yield almost identical results and outside this range the 2nd order model does not improve accuracy except in the case of predicting temperature gradients at very low velocity (< 1 m/s) and K < 0.1 °C/s . The 3rd order, 2-equation model is also not an improvement over the 1st model, and, in fact, has limited ability to predict temperature gradients due to its strong dependence on the solid-gas heat transfer coefficient in the air channel.

Figure 4 is a design map, based on this research, for the specific unit cell geometry and materials described in the March 2004 report. One way to use the map is to draw a horizontal line corresponding to the maximum allowable temperature gradient. Values of *K* and *U* below this line can be selected such that the heating time (horizontal axis) is minimized. This gives some flexibility in choosing *K* and *U* but these parameters may be limited by other system considerations such as pumping power, or heater size. Alternatively, the heating time requirement could be imposed, and then *K* and *U* selected such that temperature gradient is minimized. Use of the map in this way gives approximate values of *K* and *U*, which are an excellent starting point for performing CFD simulations of the heating/cooling process if detailed results are required.

Conclusions and Future Directions

- The FMA program was used in conjunction with the ANSYS commercial software to demonstrate a method to study structural failure in the PEN despite issues with the aspect ratios of the material layers and difficulties in performing a complex fracture analysis.

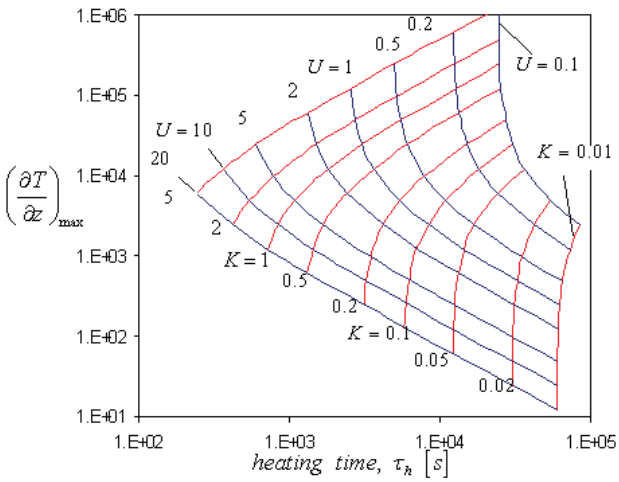

FIGURE 4. Design map showing maximum temperature gradient vs. heating time for various values of *K* and *U*. Given the maximum allowable temperature gradient, *K* and *U* can be selected such that heating time is minimized. This map is specific to the unit cell geometry and materials under consideration, and a temperature rise of 600ºC from ambient to operating temperature.

- For the global model studied, failure would most likely occur in the anode as crack growth towards the electrolyte during cooling.
- If details of the 3-D time-varying temperature fields are desired, then transient CFD modeling is required (at significant computational expense), but 2nd and 3rd order analytical models were not significantly improved over the 1st order model.
- The 1st order model may safely be used within the range of validity that was established and for the purpose of predicting total heating time, and maximum temperature gradients developed during a heating/cooling process.
- Several future possibilities for structural analysis include the study of thermal fatigue as the anode cycles between tension and compression and incorporating the impact of mechanical constraints into the failure analysis.

FY 2006 Publications/Presentations

1. Johnson, Janine and Jianmin Qu. Three-Dimensional Numerical Simulation Tools for Fracture Analysis in Planar Solid Oxide Fuel Cells (SOFCs). 2006. Cocoa Beach, FL, United States: American Ceramic Society, Westerville, OH 43086-6136, United States.

2. Johnson, Janine and Jianmin Qu, An interaction integral method for computing the stress intensity factors of planar cracks in non-uniform temperature fields. Engineering Fracture Mechanics, *submitted May 2006*.

References

1. Gosz, M., M. Dolbow, and B. Moran, Domain integral formulation for stress intensity factor computation along curved three-dimensional interface cracks. International Journal of Solids and Structures, 1998. 35(15): p. 1763-1783.

2. Nahta, R. and B. Moran, Domain integrals for axisymmetric interface crack problems. International Journal of Solids and Structures, 1993. 30(15): p. 2027-40.

3. Johnson, Janine, Fracture failure of solid oxide fuel cells, in Mechanical Engineering. 2004, Georgia Institute of Technology: Atlanta. p. 114.